Materials Science

CONJUGATE GRADIENT OPTIMIZATION TECHNIQUES

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Function optimization is a very common and necessary tool in fields as varied as machine learning, economics and engineering. One way it is relevant to materials science is in the fact that atoms in a crystalline solid tend to organize themselves into the lowest energy configuration. If a function can be created that relates the energy of a group of atoms to their configuration, then a minimization of that function will give the lowest energy configuration. These results can be compared to x-ray diffraction data on the crystal and thereby give a measure of how accurately the function models the crystal energy. In this study, several crystal test functions were optimized using two conjugate gradient methods and a brute force steepest descent method. The limiting factor in performing these calculations in most cases is computation time, therefore the number of function evaluations was the variable used to compare the methods. Several function properties that confuse the conjugate gradient techniques are pointed out and solutions are examined.